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Fred W. McLafferty

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Ab initio calculations of isomeric carbon clusters C_n^0 and C_n^+ , $n = 2-4$, yield structures and energies similar to previous reports, although five (not two) C_4^+ structures have local energy minima. Dissociative ionization of structurally varied precursors was used to prepare C_3 and C_4 ionic and neutral isomers; however, their mass spectra from collisionally activated dissociation (CAD) and neutralization-reionization (NR) under a wide variety of conditions are indistinguishable, indicating only one isomer or the same mixture of isomers. Likewise, CAD and NR spectra of C_4^+ and C_4^0 from $^{13}CH_2=CHCH=^{13}CH_2$ and C_3^+ and C_3^0 from $CH_2=^{13}CHCH_3$ show complete $^{13}C/^{12}C$ scrambling. CAD cross sections are consistent with C_4^+ - C_6^+ ions as mainly linear isomers and C_7^+ ions from cyclic precursors as mainly cyclic. Product abundances from the unimolecular dissociation of C_n^0 , C_n^- , and C_n^+ allow the selection of thermodynamic data that should be of higher relative accuracy, such as 11.4 eV for the C_3 ionization energy from reported values of 10.0-13.0 eV.

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Carbon Clusters Studied by Neutralization-Reionization Mass Spectrometry

Fred W. McLafferty

Department of Chemistry
Baker Laboratory
Cornell University
Ithaca, NY 14853-1301

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SMALL CARBON CLUSTERS (C_n^0 , C_n^+ , C_n^-) FROM ACYCLIC AND CYCLIC PRECURSORS. NEUTRALIZATION-REIONIZATION MASS SPECTROMETRY AND THEORY

The chemistry of C_n molecules and ions in plasmas (carbon arcs, laser ablation) and in the formation of polynuclear aromatics, diamond films, and soot has been the subject of extensive theoretical and experimental research. In these studies, ab initio calculations of isomeric carbon clusters C_n^0 and C_n^+ , $n = 2-4$, yield structures and energies similar to previous reports, although five (not two) C_4^+ structures have local energy minima. Dissociative ionization of structurally varied precursors was used to prepare C_3 and C_4 ionic and neutral isomers; however, their mass spectra from collisionally activated dissociation (CAD) and neutralization-reionization (NR) under a wide variety of conditions are indistinguishable, indicating only one isomer or the same mixture of isomers. Likewise, CAD and NR spectra of C_4^+ and C_4^0 from $^{13}CH_2=CHCH=^{13}CH_2$ and C_3^+ and C_3^0 from $CH_2=^{13}CHCH_3$ show complete $^{13}C/^{12}C$ scrambling. CAD cross sections are consistent with C_4^+ - C_6^+ ions as mainly linear isomers and C_7^+ ions from cyclic precursors as mainly cyclic. Product abundances from the unimolecular dissociation of C_n^0 , C_n^- , and C_n^+ allow the selection of thermodynamic data that should be of higher relative accuracy, such as 11.4 eV for the C_3 ionization energy from reported values of 10.0-13.0 eV.

Technical Reports and Journal Articles:

362. McLafferty, F.W. Neutralization-Reionization Mass Spectrometry, Int. J. Mass Spectrom. Ion Processes **1992**, 118/119, 221-235.
377. Fura, A.; Turecek, F.; McLafferty, F.W. Small Carbon-Clusters (C_n^0 , C_n^+ , C_n^-) from Acyclic and Cyclic Precursors. Neutralization-Reionization Mass Spectrometry and Theory, J. Am. Chem. Soc., submitted.

Personnel Participating in this Research:

Aberra Fura, Graduate Student, Ph.D. awarded May 1992

Frantisek Turecek, Senior Research Associate, now Professor of Chemistry,
University of Washington

Fred W. McLafferty, Principal Investigator, Professor of Chemistry

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Principal Investigator: Mass Spectrometry
Fred W. McLafferty
Mailing Address: Department of Chemistry
Baker Laboratory
Cornell University
Ithaca, New York 14853-1301
Phone Number: 607/255-4699 Fax Number: 607/255-7880
E-mail Address:

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